

# The Total Energy from X-Ray Electron Density?

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The point of N-representability is to ensure the relationship of a density matrix to an N-body antisymmetric wave function. The antisymmetry is the theoretical analog of the experimental indistinguishability of the electrons. The variational theorem used to optimize energy will only hold true if the density matrices used for such purpose are N-representable. For very large molecules, it is advantageous to have the one-body density matrix in a kernel energy method (KEM) form. Here we give the explicit form of the corresponding N-representable two body density matrix, and state how it may be used to calculate a molecular energy.

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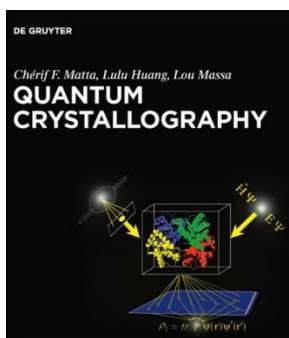


Figure 1

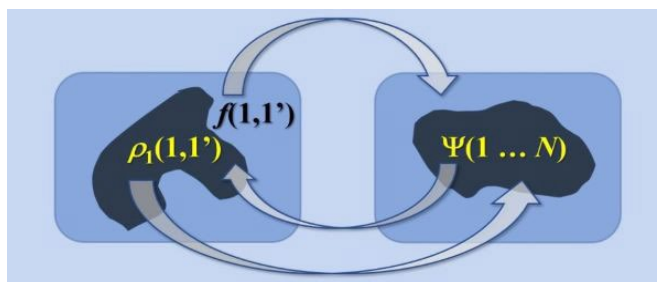


Figure 2